

# Combustion Research Facility News



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## Robert Barlow Awarded Combustion Institute's Alfred C. Egerton Gold Medal

*By Patti Koning*

Sandia National Laboratories scientist Robert Barlow was awarded the Alfred C. Egerton Gold Medal at the 35<sup>th</sup> International Symposium on Combustion in San Francisco on August 6. Given every two years by the Combustion Institute, the award recognizes “distinguished, continuing, and encouraging contributions to the field of combustion.”

Lawrence Harding of Argonne National Laboratory won the Bernard Lewis Gold Medal for “brilliant research in the field of combustion,” and Paul Clavin of Aix-Marseille Université in France won the Ya B. Zeldovich Gold Medal “for outstanding contribution to the theory of combustion or detonation.”

Robert was honored for “pioneering contributions to simultaneous laser diagnostics and their application to the understanding of turbulence-chemistry interactions in flames.” He has developed unique experimental capabilities that combine measurements of Raman scattering, Rayleigh scattering, and laser-induced CO fluorescence with crossed planar flame sheet imaging. Taken together, these measurements yield a wealth of information regarding the flame structure—including the temperature, major species, mixture fraction, reaction progress, and the gradients of these quantities—with high precision and spatial resolution.

This work is leading to an improved understanding of the fundamental nature of turbulent combustion, which, in turn, helps provide detailed data sets for developing and evaluating computer models that



*Robert Barlow, left, with former Sandian and current research collaborator Simone Hochgreb of the University of Cambridge, who presented him with the Alfred C. Egerton Gold Medal at the 35<sup>th</sup> International Symposium on Combustion. (Photo courtesy of Knight Lights)*

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## Robert Barlow awarded Combustion Institute's Alfred C. Egerton Gold Medal (cont'd)

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Robert Barlow accepting his  
Alfred C. Egerton Gold Medal.  
(Photo courtesy of Knight Lights)

will eventually be used to design advanced combustion systems for transportation and power generation. Robert is also well-regarded in the combustion community as an advocate for international collaborative research and the main organizer of the Turbulent Nonpremixed Flames workshop series on the measurement and computation of turbulent flames.

"This is a significant honor that is both thrilling and humbling because there are many people who contributed to the body of work that is being acknowledged, and there is a lot more work to be done," says Robert.

Robert is the second Sandia employee to be awarded a Gold Medal by the Combustion Institute. Jim Miller, now retired, won the Bernard Lewis Gold Medal at the 31<sup>st</sup> International Symposium on Combustion in Heidelberg, Germany.

Robert received his Ph.D. and M.S. in mechanical engineering from Stanford University and his B.A. in chemistry from Amherst College. He was a program co-chair for the 34<sup>th</sup> International Symposium on Combustion (Warsaw, 2012) and served as editor of the *Proceedings of the Combustion Institute* (2003–2007). He is an editorial board member of *Combustion Theory and Modelling* (1996–present) and is a past editorial board member of *Progress in Energy and Combustion Science* (2002–2004).

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# 35<sup>TH</sup>

## INTERNATIONAL SYMPOSIUM ON COMBUSTION SAN FRANCISCO



**T**he 35<sup>th</sup> International Combustion Symposium, the premier conference on combustion science and application held on August 3–8 in San Francisco, was a resounding success thanks to Sandia's Combustion Research Facility. More than 1,500 researchers gathered from around the world to discuss the latest innovations in understanding and predicting combustion-related phenomena, approximately 250 more than had ever previously attended this biennial event.

Elaine Oran, a professor of engineering at the University of Maryland, gave the keynote address. The event also included four invited plenary talks, 435 oral presentations, and 690 posters describing cutting-edge fundamental and applied combustion research.

Jonathan Frank and Chris Shaddix served as co-chairs of colloquia on Turbulent Flames and Heterogeneous Combustion. CRF researchers authored or co-authored 33 oral presentations. In addition,

Robert Barlow was awarded one of the three Gold Medals for distinguished career achievement offered biennially by the Combustion Institute, which sponsors the Symposium.

CRF researchers also helped organize three different technical workshops held just before the start of the Symposium:

- Robert Barlow organized the Turbulent Nonpremixed Flames (TNF) workshop.
- Chris Shaddix organized the International Sooting Flame (ISF) workshop.
- Nils Hansen organized the Flame Chemistry Workshop.

The TNF and ISF workshops also included optional CRF lab tours, which were enjoyed by 70 workshop participants. The symposium itself was largely organized by Sandia, with Chris Shaddix, Jackie Chen, and Melissa Betz leading the local organizing committee. Judit Zádor and Ahren Jasper organized the contributed posters.

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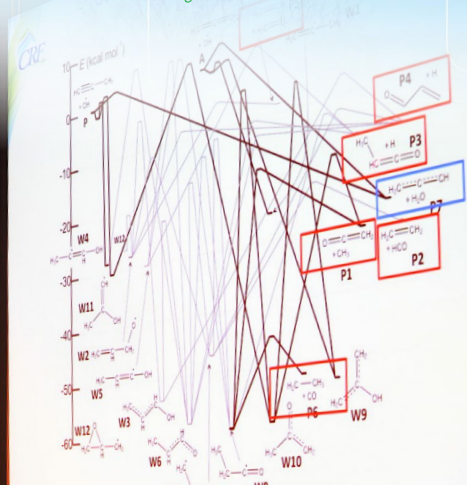


## Symposium (cont'd)

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Judit Zádor presents "Adventures on the  $C_3H_5O$  potential energy surface: OH + propyne, OH + allene and related reactions," research conducted with James A. Miller of Argonne National Laboratory. Sandia researchers authored or co-authored 33 of the 435 oral presentations given at the event. (Photos by Dino Vournas)



Elaine Oran, a professor of engineering at the University of Maryland, gave the keynote address on "Understanding explosions: From catastrophic accidents to the creation of the universe."



Katharina Kohse-Höinghaus, president of the Combustion Institute and a professor at the University of Bielefeld, opens the 35<sup>th</sup> International Symposium on Combustion, which was held in San Francisco on Aug. 3-8.

# 35<sup>TH</sup> INTERNATIONAL SYMPOSIUM ON COMBUSTION SAN FRANCISCO





# CRF Reunion Luncheon Brings Together Staff, Retirees, Postdocs, and Visitors

By Patti Koning

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With more than 100 visiting researchers each year, many paths cross at the Combustion Research Facility. The CRF reunion luncheon, held during the 35<sup>th</sup> International Symposium on Combustion in San Francisco the first week of August, brought together a number of current staff, retirees, past and present postdocs, and other visitors.

Three CRF directors were in attendance—current director Bob Hwang; recently retired Bob Carling (2008–2013); and Bill McLean, who led the CRF from 1993–2005. “This is a chance to see a lot of old friends and colleagues who I don’t see so often,” said McLean. “Plus it’s interesting to hear about the new research. We’ll never run out of technical challenges to solve.”



CRF directors past and present: Bob Carling (2008–2013), Bob Hwang (current), and Bill McLean (1993–2005).

While CRF postdocs occasionally move onto staff positions at Sandia, most leave for permanent research positions in industry, at government or private research institutes, or as faculty members at universities across the globe. The reunion luncheon brought together the “family” of Nils Hansen, Ahren Jasper (both CRF researchers), and Stephen Klippenstein, a Distinguished Fellow at Argonne National Laboratory. Klippenstein was a CRF researcher before joining Argonne, and Jasper was previously Klippenstein’s postdoc at Argonne before coming to the CRF. The three researchers are frequent collaborators.

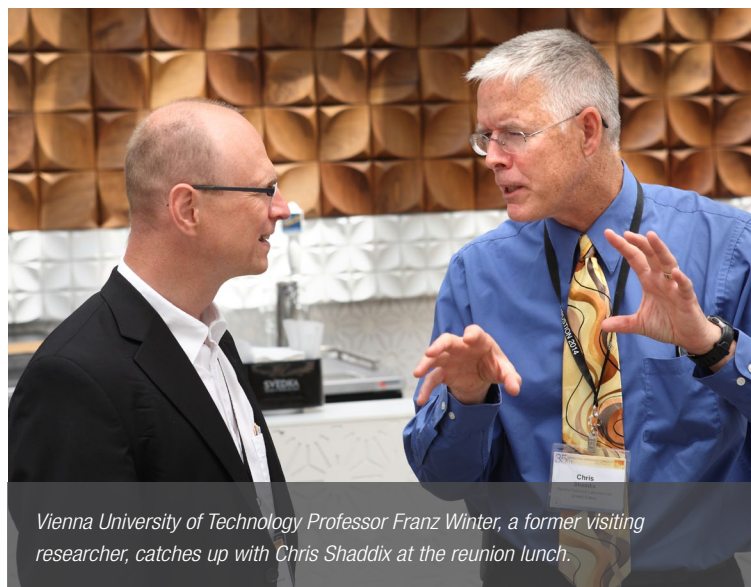
Hong Im travelled all the way from Saudia Arabia, where he is a professor at the Clean Combustion Research Center (CCRC) at King Abdullah University of Science and Technology. He was a postdoc



Hamming it up for the camera are (from L-R) CRF researchers Ethan Eagle and Mark Musculus; Sebastian Kaiser, a professor at the University of Duisburg-Essen and a former postdoc and Sandia staff member; and Gilles Bruneaux of France’s IFP Energies nouvelles (IFPEN). (Photos by Dino Vournas)

of Jackie Chen from 1996 to 1999 before becoming a professor at the University of Michigan. “The CRF was a great start for a career in academics,” he said. “Now the CCRC is trying to become the CRF of the Middle East.”

Matthew Campbell was probably the newest CRF researcher at the party. He had just completed his first week as a Sandia postdoc for Hope Michelsen. “Everyone has been very welcoming,” he said. “This party gives me the opportunity to meet a lot of successful CRF researchers face to face, people I’m familiar with through their work.”



Vienna University of Technology Professor Franz Winter, a former visiting researcher, catches up with Chris Shaddix at the reunion lunch.



## CRF Researchers Honored by DOE

By Holly Larsen

The Annual Merit Review and Peer Evaluation Meeting held on June 17, 2014, gave two DOE groups, the Hydrogen and Fuel Cells Program and the Vehicle Technologies Office, an opportunity to recognize exceptional achievement in specific areas. The CRF is especially pleased that retiring manager Dennis Siebers was honored with a Distinguished Achievement Award from the Vehicle Technologies Office “for lifetime achievement in understanding engine combustion and emissions processes, leading to cleaner, more efficient engines worldwide.” This award is a fitting acknowledgment of Dennis’s significant impact on and contribution to combustion science over the course of his career.

In addition, the Hydrogen and Fuel Cells Program recognized Sandians Brian Somerday and Chris San Marchi for outstanding achievements in hydrogen materials compatibility with a Program Area Award for Hydrogen Production and Safety, Codes, and Standards. Brian leads a research collaboration with Kyushu University that is developing predictive models for hydrogen embrittlement in metals and serves as Sandia’s lead of the newly launched H<sub>2</sub>FIRST project, which provides the science and engineering to advance a reliable and economic refueling infrastructure for hydrogen vehicles. Chris has been an integral part of numerous codes and standards development committees and has created several references on materials compatibility, including Sandia’s *Technical Reference*—the first hydrogen-specific reference from the Fuel Cell Technologies Office (FCTO) to be incorporated into President Obama’s Open Energy Information Initiative.

“I join the entire CRF team in congratulating these Sandians for their excellent work,” said Bob Hwang, director of Sandia’s Transportation Energy Center, which includes the CRF. “Recognition from peers is a highlight for any career, and these awards are highly deserved and greatly appreciated.”



Two Sandians received the DOE Hydrogen and Fuel Cell Program achievement award. Pictured (from left to right) are Erika Sutherland (DOE FCTO), Brian Somerday, Chris San Marchi, and Will James (DOE FCTO).

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## SAE International Honors CRF Researchers for Outstanding Presentations

By Holly Larsen

Solid technical work is great—but the ability to communicate effectively about that work is equally critical. To acknowledge the importance of good communication—and maintain a high quality of presentation at its technical meeting—SAE International established the SAE Excellence in Oral Presentation award in 1972.

This year, two Sandians, Joseph Oefelein and Lyle Pickett, were honored with this award for outstanding presentations offered at the 2014 SAE World Congress, placing them among the top 5% of presenters at this highly attended event. Awards are based on the evaluations of attendees at each technical session.

Joseph’s presentation, “*Effects of Real-Fluid Thermodynamics on High-Pressure Fuel Injection Processes*,” highlighted his recent work with Sandians Guilhem Lacaze, Rainer Dahms, and Anthony Ruiz and with Antony Misdariis of Renault SAS.

In his presentation, “*Comparison of Near-Field Structure and Growth of a Diesel Spray Using Light-Based Optical Microscopy and X-Ray Radiography*,” Lyle described recent research he’d conducted with fellow Sandian Julien Manin and with Alan Kastengren and Christopher Powell, both of Argonne National Laboratory.

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## SAE International Honors CRF Researchers for Outstanding Presentations (cont'd)

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The CRF congratulates Joseph and Lyle for this honor, and commends the teams that contributed to the technical work presented.



Joseph Oefelein



Lyle Pickett

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## Paul Miles Appointed Manager of Engine Combustion Department

by Holly Larsen



Paul Miles

On June 6, Paul Miles became manager of the CRF's Engine Combustion Department, which focuses on building the science base needed by industry to develop new generations of high-efficiency, clean engines. He took the helm from departing manager Dennis Siebers, who recently retired from Sandia National Laboratories.

Paul brings a wealth of experience to his new role. He has actively researched flow, mixing, and combustion processes in reciprocating engines since 1992. As a Distinguished Member of the Technical Staff, Paul has been leading the light-duty diesel engine research program at the CRF since 1997.

Further, Paul is a Fellow of SAE International and has been honored with the SAE Horning, Myers, and McFarland awards. He also serves on the advisory committees of several international conferences and is a past co-chair of the SAE Powertrain, Fuels, and Lubricants activities.

Paul has a track record of multitasking at the international level. In addition to fulfilling his responsibilities at the CRF, Paul is an adjunct professor in the Department of Energy Sciences at Lund University in Sweden and has a guest professor appointment at the School of Advanced Optical Technologies at Friedrich-Alexander University in Erlangen, Germany.

Speaking of his new role, Paul said, "I'm looking forward to helping this group continue to make exceptional contributions to our understanding of engine combustion. The CRF engine group has a world-class staff and it is a privilege to work with them."



# Dennis Siebers Leaves Behind a Lasting Legacy in Engine Combustion Research

By Patti Koning

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Nearly 40 years ago, Dennis Siebers was drawn to Sandia for the opportunity to perform “exceptional service in the national interest.” In July, his 38-year career at Sandia, most of it spent in the CRF, came to a close with his retirement.

“It’s difficult to measure the impact that Dennis has demonstrated over several decades of work in engine combustion,” said Bob Carling, who retired as director of the CRF last year. “From designing and building sophisticated experiments to leading and managing the top group of engine research scientists and engineers in the world, he has shown excellence in everything he has undertaken. His quiet, unassuming manner will be missed by all he has touched.”

Gurpreet Singh, program manager for DOE’s Advanced Combustion Engines Program, describes working with Dennis as a great pleasure. “He has made numerous contributions to the combustion community and managed a program that has put DOE’s engine combustion research at the forefront. His efforts have resulted in improved fuel economy for cars and trucks, saving the nation billions of gallons of fuel and avoiding millions of tons of emissions.”

In June, Dennis’s impact and contributions were recognized at the DOE 2014 Annual Merit Review and Peer Evaluation Meetings for the Hydrogen and Fuel Cells Program and the Vehicle Technologies Office. The Vehicle Technologies Office presented Dennis with a Distinguished Achievement Award “for lifetime achievement in understanding engine combustion and emissions processes, leading to cleaner, more efficient engines worldwide.”

Dennis joined Sandia in 1976 after completing his B.S. and M.Sc. in mechanical engineering at Purdue University. One of the first projects he worked on was Solar One, the country’s first large-scale thermal solar power plant located in the Mojave Desert. Bob was one of his colleagues on that project.

“This was an early highlight of my career,” said Dennis. “I worked on the thermal analysis of the contractor-designed central receivers for the power plant, providing independent analyses of the various

designs for Sandia. For someone right out of school, this was pretty exciting, especially having the opportunity to eventually go up on top of the tower and see the project firsthand.”

After three years at Sandia, Dennis was back in school at Stanford University to earn his Ph.D. in mechanical engineering through Sandia’s Doctoral Studies Program. When he graduated in 1982, he began working in the CRF, which was still in its early years.

“I didn’t have an extensive background in combustion at the time, so for the first few years I worked pretty frantically to come up to speed in the field and contribute to the programs,” Dennis recalled. “It was a very exciting and dynamic time.”



Dennis Siebers

In 1989, he became manager of the Combustion Applications Department, a position he held for two years before returning to research full-time. “I was thinking about management early in my career, so when an opportunity came up to become acting manager, I took it,” he explained. “That turned into two years. I enjoyed it, but I also realized I wanted more to my technical career and to continue pursuing research.”

Bob took over the management role, leaving Dennis free to continue building a new CRF capability: the constant-volume combustion vessel for studying engine combustion processes under well-controlled conditions. “This was a time when we were trying to assemble engine experiments that more

closely approximated real engines,” said Bob. “However, Dennis was prescient enough to know that our lab engines were a challenge for the nascent community of engine modelers.”

Dennis designed the combustion vessel to enable many different types of fundamental engine-related combustion and noncombustion experiments. This led to one of his key contributions to the field of combustion: understanding fuel sprays and their impact on engine combustion processes.

“The scaling law that he developed for diesel sprays is widely used by industry and research groups worldwide and is essentially the standard for describing diesel fuel-jet penetration and mixing and

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## Dennis Siebers Leaves Behind a Lasting Legacy in Engine Combustion Research (cont'd)

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how it is affected by parameters such as boost pressure, gas temperature, injection pressure, and orifice diameter—critical information for diesel-engine designers and researchers,” said Senior Scientist John Dec.

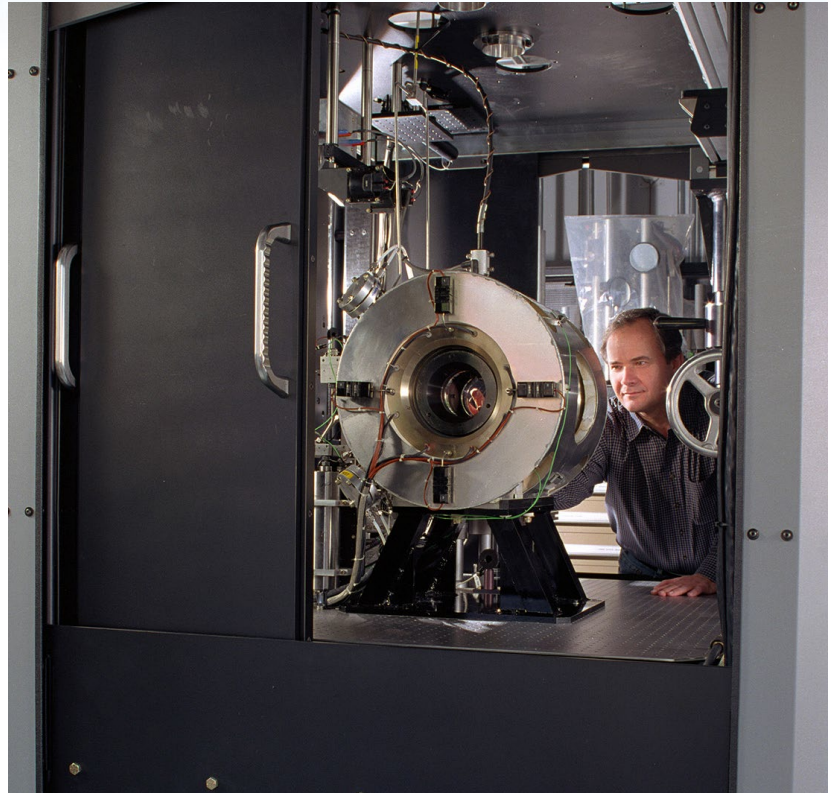
Lyle Pickett took over this research when Dennis returned to the role of manager of the Engine Combustion Research Department in 2002. Lyle also formed the Engine Combustion Network (ECN) in response to the increasing demand from the combustion community for the fundamental fuel-spray research that Dennis and his research team, which included Lyle, had developed over the prior decade. Initially, the ECN’s purpose was to provide the Sandia database to the external community via the web; it has since gone on to become the focal point for global collaboration among experimental and computational researchers in engine combustion.

“It’s been a privilege to work with Dennis. He’s really shaped my career,” said Lyle. “I’m still using the lab that he built over 20 years ago, which is quite remarkable.”

As manager, Dennis developed strong working relationships with DOE sponsors and industrial partners in the auto and diesel-engine industries, which provided the opportunity to triple the funding for the department. He also helped establish and maintain the CRF’s reputation as the leader in the worldwide engine combustion community.

“He excelled at all aspects of managing the department,” said John. “His leadership allowed us to keep a strong focus on our research. Moreover, he made it a priority to be available as a mentor and to promote the careers of those whom he managed, through various internal and external award nominations and to ensure that people were promoted within Sandia as their accomplishments warranted.”

Dennis described this role as a mentor and guide to staff and technologists as a highlight of his time as a manager. “I think this was one of my strongest points as a manager,” he said. “And now the work that consumed much of my career is in good hands. I have every confidence that Paul Miles will take this department in new directions with significant new accomplishments and continued excellence.”



*Dennis Siebers examines an equipment installation for the CRF’s Diesel Simulation Facility.*



*2012 SAE President Frank Klegon and John Johnson, Michigan Technological University, present the 2011 SAE John Johnson Award for Outstanding Research in Diesel Engines to Lyle Pickett, Cherian Idicheria, Caroline Genzale, and Dennis Siebers.*



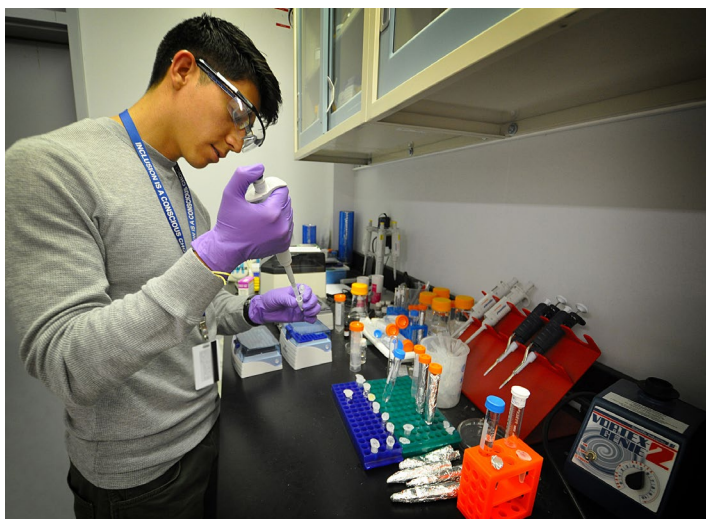
# Students and Professors Spend the Summer at Sandia under DOE's WDTS Program

By Holly Larsen

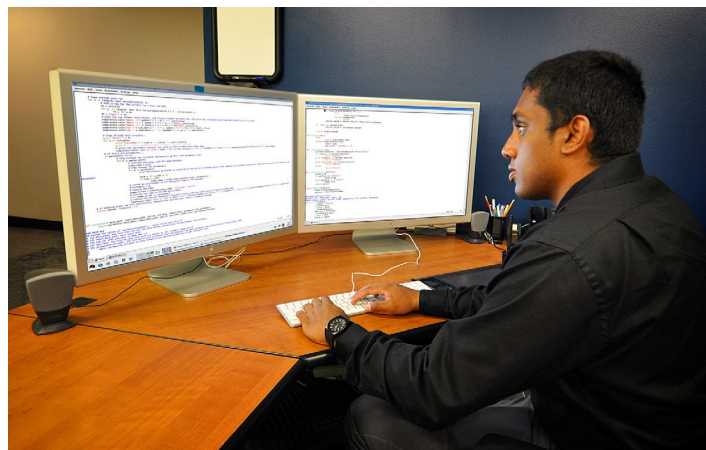
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This past summer, the CRF was the research home to 11 students and 2 professors who participated in the DOE Office of Science's Workforce Development for Teachers and Scientists (WDTS) Program. By allowing students and professors to conduct research internships at national laboratories, this program is helping to develop the next generation of scientists, teachers, and engineers.

For example, under mentor Bert Debusschere, California State University, Stanislaus student Kathryn Dahlgren explored the viability of different algorithms for resilient partial differential equation solvers for combustion modeling. On a summer break from California State Polytechnic University, Pomona, Christopher Nilsen studied ducted



Eduardo Valle worked with mentor Dr. Carl Hayden to help identify novel drug delivery methods.



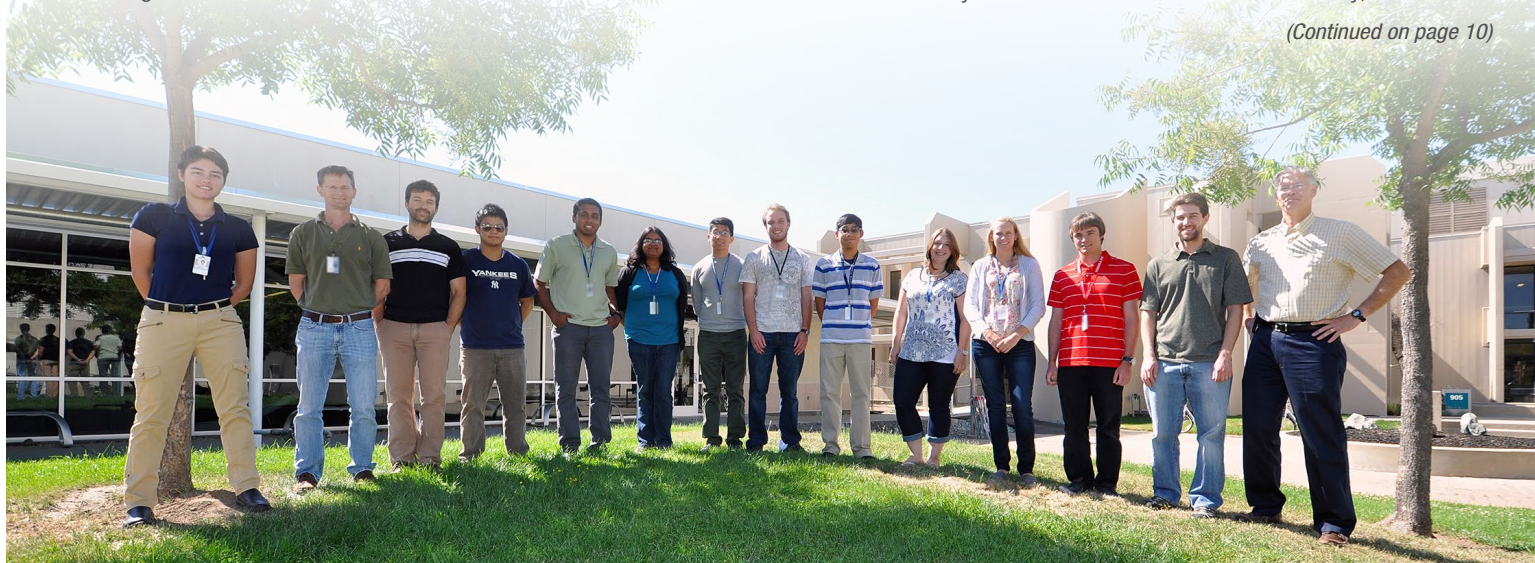
Over the summer, Raj Kumar of Las Positas College worked on uncertainty in large-eddy simulations with mentor Jeremy Templeton. (Photos by Daniel Strong)

The 10 undergraduate students who spent their summer at the CRF hail from as far as Vermont and as close as Livermore. Their work is contributing to efforts to advance clean and efficient fuel and vehicle technologies across the CRF.

fuel injection, a means of reducing soot in compression-ignition engines, with mentor Chuck Mueller. And Ashley Scully of Saint Michael's College in Vermont studied Criegee intermediates in reaction with tropospheric compounds under mentor Leonid Sheps.

The CRF also hosted a WDTS duo from the University of the Pacific—Ph.D. student Kyle Covert and Professor Balint Sztaray, whose

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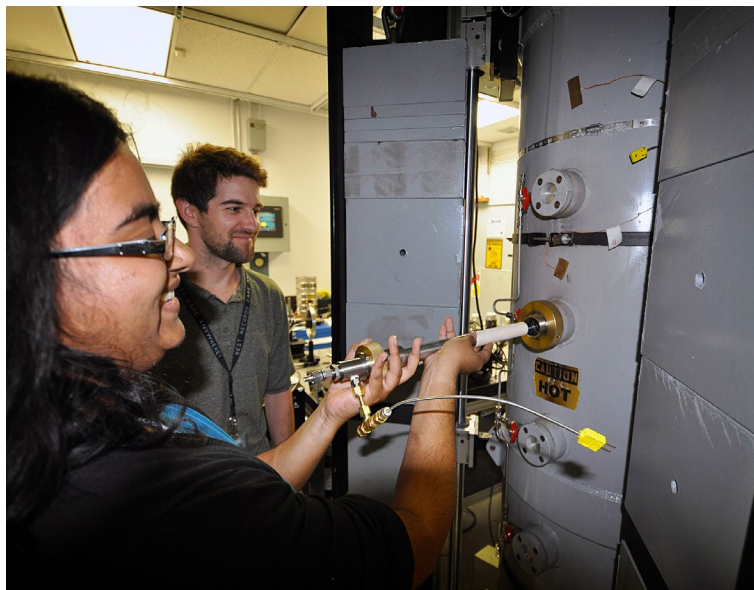




## Students and Professors Spend the Summer at Sandia under DOE's WDTs Program (cont'd)

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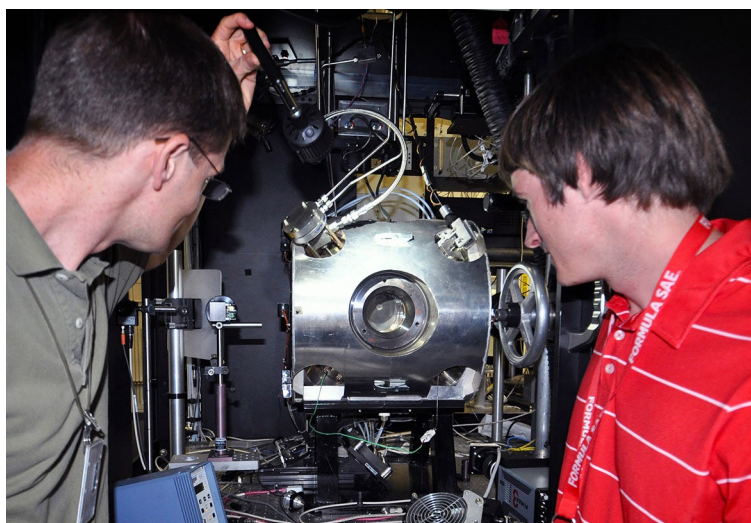
*Under the supervision of mentor Ethan Hecht, Samira Iqbal of Las Positas College worked on a reactor that is used to characterize the kinetics of pulverized coal oxy-combustion under pressure.*

work with David Osborn is described on page 11—as well as Dr. Jennie Guzman, assistant professor of physics at California State University, East Bay. Dr. Guzman collaborated with Lori Culberson and Dave Chandler on new experiments to image high-resolution spectroscopy and photophysics associated with atomic transitions such as Rabi cycling and AC Stark shifting of energy levels.

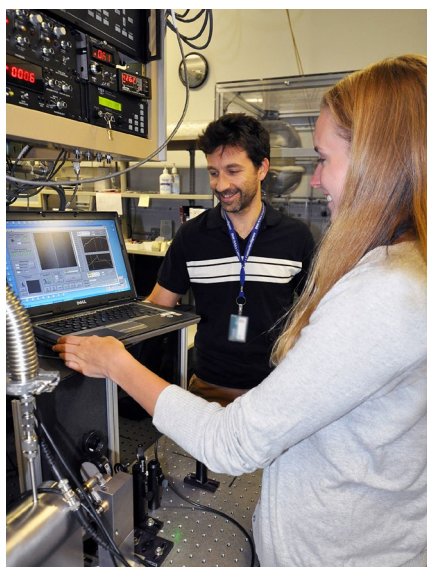
The students were enthusiastic about their time at Sandia. “I’m really grateful that my mentors have put emphasis on teaching me and ensuring that I have not only a productive learning experience, but also an enjoyable one,” said Brittany Hagler, a student at Union University in Tennessee. She worked with Habib Najm and Kamaljit Chowdhary to improve the calibration of the Arrhenius rate equation, which is used to predict the ignition times of combustion engines.

Samira Iqbal, a Las Positas College student working under mentor Ethan Hecht, said she loves getting hands-on practice in the lab—in this case, working with a reactor that is used to characterize the oxy-combustion kinetics of pulverized coal under pressure. She added, “It’s great seeing how the work that I’m doing in the CRF can apply to a bigger picture for energy research.”

The students' enthusiasm is shared by CRF staff. “The CRF is delighted to welcome the WDTs students and professors,” said Senior Manager Dawn Manley. “The program has been instrumental in enriching the research experiences of the students, professors, and our CRF staff. We’re proud to help shape the next generation of teachers and scientists and hope to support this program for many years to come.”



*WDTs intern Christopher Nilsen worked with mentor Chuck Mueller on a project that examined fuel injection through a duct to reduce soot emissions from compression ignition engines.*



*Ashley Scully studied Criegee intermediates in reaction with tropospheric compounds under mentor Leonid Sheps (on left).*

***The 2015 WDTs program is now accepting applications. See [crf.sandia.gov](http://crf.sandia.gov) for more information.***



# VFP Professor Balint Sztaray Continues CRF Collaboration

By Holly Larsen

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Over the past two summers and a sabbatical semester in 2013, University of the Pacific (UOP) chemistry professor Balint Sztaray and his research group have been working with the CRF's David Osborn on a project to improve the selectivity of the current multiplexed gas-phase chemical kinetics instrument. Specifically, the two researchers are focusing on developing a new instrument that combines Balint's method of photoelectron-photoion coincidence spectroscopy with David's multiplexed photoionization mass spectrometry (PIMS).



Balint Sztaray

DOE has been a partner in this effort, providing funding to Balint through its Visiting Faculty Program (VFP). Part of the larger Workforce Development for Teachers and Scientists (WDTs) Program run by DOE's Office of Science, VFP is designed to increase research competitiveness by enabling a college or university faculty member and up to two students to conduct 10 weeks of collaborative research with national laboratory staff.

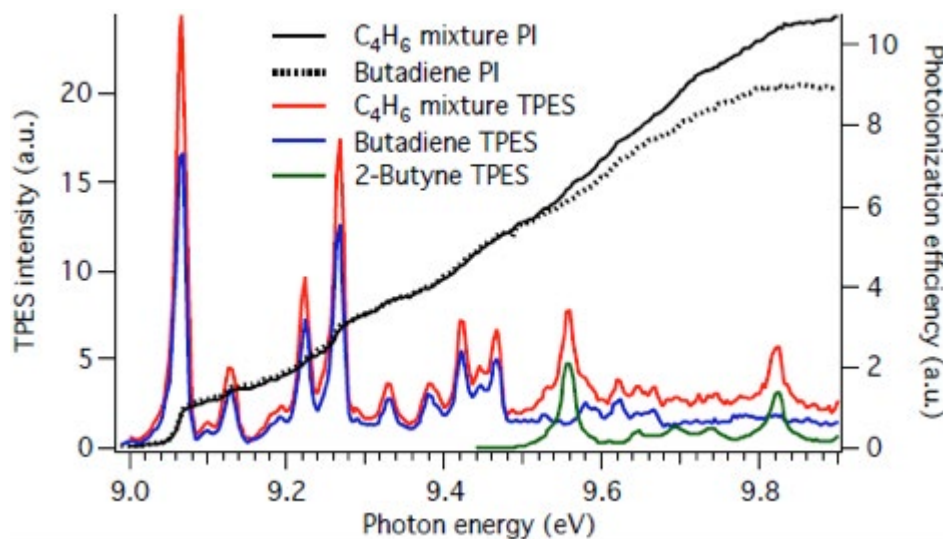
As a returning VFP award recipient, Balint was back at the CRF this past summer along with UOP Ph.D. student Kyle Covert, to work with David on bringing their concept closer to reality. Their work to date, which included a trip to Switzerland to run experiments on a unique endstation at the Swiss Light Source (SLS), was described in detail in a proof-of-concept paper published in the prestigious *Journal of Physical Chemistry Letters*.

PIMS, which applies tunable synchrotron light to enable isomer separation based on unique photoionization spectra, is a powerful method for time- and space-resolved chemical analysis of reactants, intermediates, and products. However, when three or more isomers are present, identification by photoionization spectra alone can be challenging.

Through experiments at SLS, the researchers showed that imaging photoelectron-photoion coincidence (iPEPICO) spectroscopy—which measures photoelectron spectra corresponding to each cation mass-to-charge ( $m/z$ ) ratio—provides a more detailed spectral fingerprint than does photoionization spectroscopy. Figure 1 shows the additional information available from the iPEPICO approach.

"David and I built on these preliminary results and, with Kyle's assistance, designed a testbed experiment to fit into the existing iPEPICO endstation at the VUV [vacuum ultraviolet] beamline of the SLS," said Balint. The team plans to travel to SLS to test a prototype design. Afterwards, they will design and build a new apparatus for the chemical dynamics beamline of the Advanced Light Source at Lawrence Berkeley National Laboratory, the planned successor of the current very successful multiplex PIMS instrument.

It was great to have Balint back at the CRF to continue this project," said David. "And we appreciate DOE's support of Balint and Kyle through the Visiting Faculty Program. This collaborative work will bring us closer to identifying all the species present in combustion reactions so that the CRF can continue to contribute to cleaner and more efficient engines."



This graph highlights the rich information offered by the proposed iPEPICO method. It shows the threshold photoelectron spectrum (TPES) of a butadiene/2-butyne mixture (red curve), together with the individual TPES spectra (blue and green curves). Also provided are the photoionization spectra of the mixture (black curve) and of butadiene (dotted line).

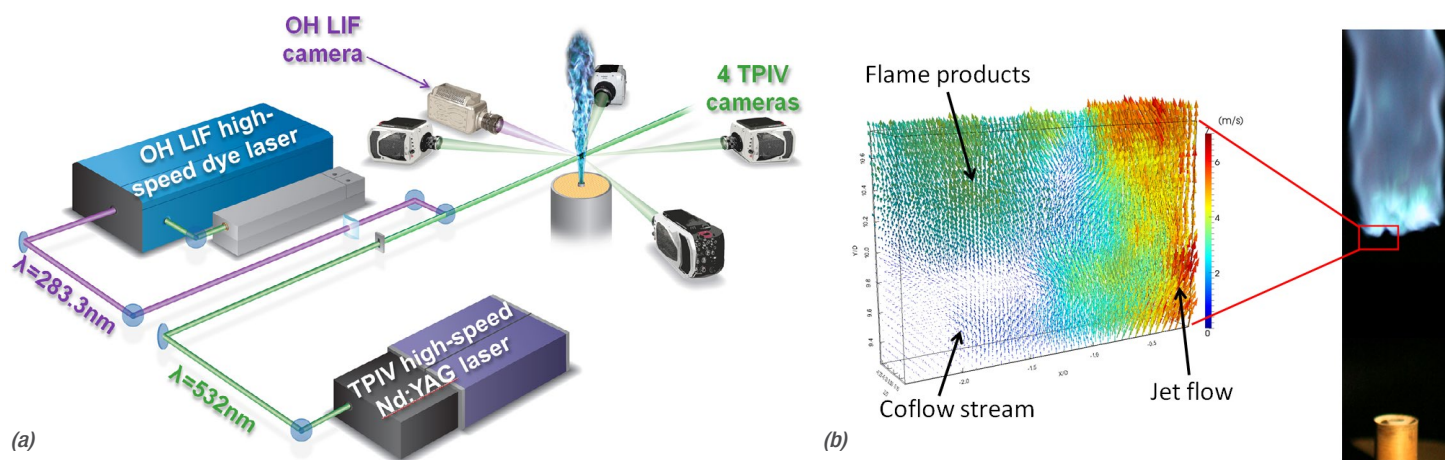
# New Diagnostic Capability Provides 3-D Measurements of Turbulent Flame Dynamics Using High-Repetition Rate Tomographic Particle Image Velocimetry

By Jonathan Frank

Capturing turbulence–flame interaction structure and studying time–history effects requires high-speed volumetric measurements performed at repetition rates sufficiently fast to resolve the relevant flow time scales. Advances in the CRF's imaging diagnostic capabilities are overcoming these challenges to provide a more complete picture of the structure and dynamics of turbulence–flame interactions.

The Advanced Imaging Laboratory has developed the capability for multi-kHz volumetric velocity-field measurements in flames. This capability is particularly valuable for studying fluid-dynamic strain

strain-rate components, and tensor invariants. (In contrast, 2-D PIV techniques provide incomplete or biased measurements of these quantities in the presence of 3-D flow structures.) Volumetric three-component velocity data are critical for the proper interpretation and analysis of high-speed imaging measurements in turbulent flows because 3-D motion can complicate temporal data-sequence interpretation. However, high-speed TPIV measurements in turbulent flames are complicated by several factors: significant variations in particle-seeding density, imaging noise, beam-steering from the index-of-refraction gradients, and the requirements for high framing rates.



**Figure 1.** (a) Experimental configuration for simultaneous high-repetition-rate TPIV and OH-LIF imaging measurements for studying turbulent-flame dynamics. (b) Single-shot three-dimensional velocity vector field from a TPIV measurement in the stabilization region of a lifted jet flame. Velocity vectors are color-coded according to their magnitudes. For the sake of clarity, 1 out of 64 vectors is displayed. The main jet flow is on the right-hand side, and the lifted flame is stabilized toward the upper left of the probe volume.

field evolution, which plays a central role in turbulence–flame interactions. Jonathan Frank and Bruno Coriton, in collaboration with CRF visitor Adam Steinberg of the University of Toronto, recently demonstrated high-repetition-rate tomographic particle image velocimetry (TPIV) feasibility for measuring the dynamics of flow–flame interactions in lifted and burner-stabilized jet flames.

The TPIV technique provides volumetric, three-component velocity-field measurements and enables access to the complete velocity-gradient tensor, which serves as the basis for determining key fluid-dynamic quantities, such as the divergence, vorticity, principal

## Experimental Method

A new experimental configuration in the Advanced Imaging Laboratory combines high-repetition-rate TPIV and hydroxyl (OH) laser-induced fluorescence (LIF) imaging (shown in Figure 1a) to improve turbulent-flame dynamics analysis. For the TPIV measurements, the particle-laden flow field is illuminated by a several-mm-thick laser sheet from a high-repetition pulsed laser. Laser light scattered by submicron aluminum oxide particles is simultaneously imaged onto four high-speed complementary metal-oxide semiconductor (CMOS) cameras with different viewing angles.

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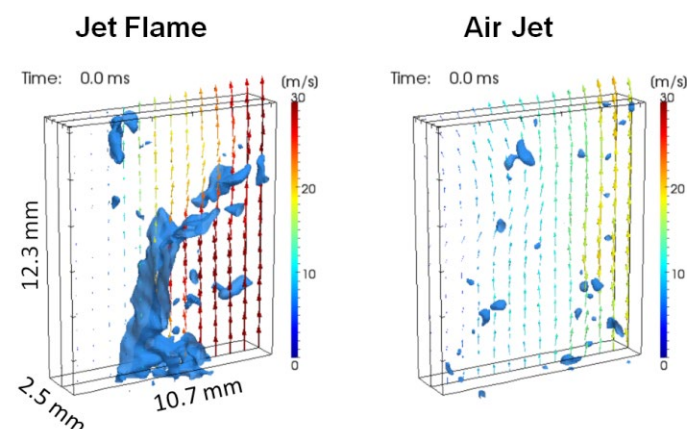


# New Diagnostic Capability Provides 3-D Measurements of Turbulent Flame Dynamics Using High-Repetition Rate Tomographic Particle Image Velocimetry (cont'd)

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Each camera captures each laser pulse's particle scattering on a single frame. The fields of view from the different cameras are carefully registered using a reference target, and a tomographic reconstruction of the 3-D particle field is performed using a multiplicative algebraic reconstruction tomography (MART) algorithm. Interframe particle displacements are determined by performing multiple-pass cross-correlation analysis using a final interrogation region size of  $24 \times 24 \times 24$  voxels ( $360 \times 360 \times 360 \mu\text{m}^3$ ), yielding more than 900,000 vectors in the probe volume for 10-kHz measurements. Figure 1b shows a single-shot velocity-field measurement at the base of a lifted dimethyl-ether (DME) jet flame.



**Figure 2.** Temporal evolution of velocity and strain-rate fields in turbulent-jet flame and nonreacting air jet from 10-kHz TPIV measurements. Blue surfaces are isosurfaces of the strain rate norm  $|s| = 8 \times 10^3 \text{ s}^{-1}$ . Velocity vectors are shown only in the midplane (1 out of 16 in-plane vectors displayed).

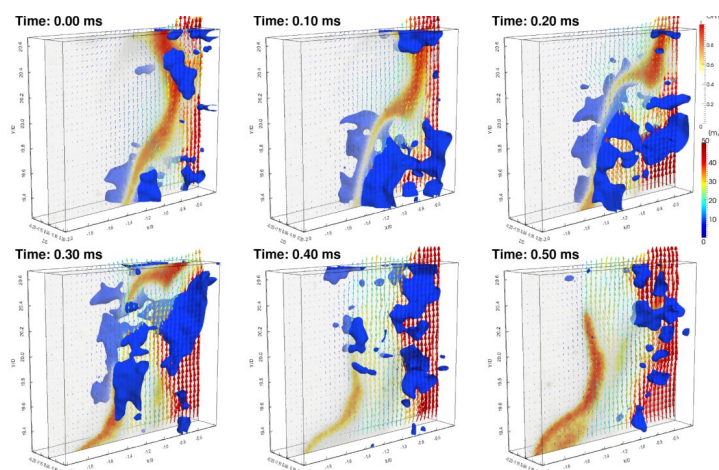
## Structure of Strain Rate Field in Turbulent Jet Flames and Nonreacting Jets

A comparison of 10-kHz TPIV measurements in a turbulent jet flame and a nonreacting air jet reveals the effects of heat release on the structure of the strain-rate field, as shown in Figure 2. In the flame, the isosurfaces of the strain rate norm,  $|s|$ , form elongated structures that are concentrated in the shear layer and span a large portion of the probe volume. In contrast, the air jet has smaller structures distributed over a broader region of the jet flow. In both cases, these high strain-rate regions are temporally intermittent, as seen in the movie sequences.

In the flame, the bursts of high strain-rate regions can lead to localized extinction. The measurement sequence in Figure 3 shows the temporal evolution of the velocity, compressive principal strain

rate, and OH-LIF fields during a localized extinction event. The velocity and OH-LIF signal are displayed in the central plane, and the compressive strain rate,  $\Gamma_o$ , is represented by blue isosurfaces at  $\Gamma_o = -15 \times 10^3 \text{ s}^{-1}$ . The onset of extinction occurs at time  $t = 0.20 \text{ ms}$  and is identified by the formation of a discontinuity in the contour of the OH-LIF signal.

The image sequence shows large coherent structures with high compressive strain rates in the localized extinction region. These structures remain coherent and closely coupled to the reaction zone until extinction occurs. As the flame approaches extinction, the high-temperature reaction zone becomes thinner. Once the flame is locally quenched, the strain rate decreases, and the large coherent structures break apart. The residence time of the extinguished region within the probe volume is  $\sim 0.5 \text{ ms}$ , which is too short to capture a subsequent reignition.



**Figure 3.** Temporal evolution of velocity and strain-rate fields during a localized extinction event in a turbulent partially premixed DME/air jet flame from simultaneous TPIV and OH-LIF imaging measurements at 10 kHz. Blue surfaces are isosurfaces of the compressive strain rate for  $\Gamma_o = -15 \times 10^3 \text{ s}^{-1}$ . Velocity vectors are shown in the same plane as the OH-LIF images (1 out of 16 in-plane vectors)

Strain-induced localized extinction is a key process in turbulent combustion that affects flame stability, emissions, and the operating conditions of practical combustion devices. The ability to capture the flow field's temporal evolution in 3-D during localized extinction is an essential tool for understanding turbulent combustion's complex dynamics. Ongoing efforts are using this new diagnostic capability to investigate the dynamics of the vorticity and strain fields in turbulent flames with localized extinction.

# ACME: Climate Modeling Powered by DOE Supercomputers, Tamed by Uncertainty Quantification

By Holly Larsen

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Facing increasing evidence of climate change, scientists around the world are working to improve climate modeling, hoping to provide decision makers solid projections to guide the development of mitigating policies. Khachik Sargsyan is leading a Sandia effort to strengthen climate models through uncertainty quantification (UQ) for the Accelerated Climate Model for Energy (ACME) program.

The DOE Office of Science recently launched ACME in an effort to integrate different models and ensure that modeling efforts benefit from the enormous computing power of DOE's leadership-class facility computers. This initiative is making extensive use of DOE supercomputers to consolidate several multi-lab projects into a single integrated and enhanced program.

"ACME consolidates a number of previous efforts and focuses on performing ultrahigh resolution modeling of fully coupled earth-ocean-atmosphere systems to predict climate change effects out to 2050," explains Chris Shaddix, manager of the Reacting Flow Research group.

Eight national labs are contributing to this effort. The end goal is to develop the most accurate climate change predictions yet, as well as investigate key fundamental science questions, such as the interaction of clouds and climate and the role of secondary organic aerosols. In addition to Khachik, Sandians involved include Andrew Salinger, who is providing software engineering expertise, and Mark Taylor. In addition to acting as the project's computational chief scientist, Mark is supporting both the atmospheric modeling task and numerical method development, targeting high-performance computing systems.

Further, ACME research is closely related to the Intergovernmental Panel on Climate Change (IPCC), a leading international authority on climate change established by the United Nations and World

Meteorological Organization in 1988. IPCC distills the latest climate science from around the world to create reports specifically intended for policy makers. As ACME simulation results become available, they will be taken into account by IPCC and will certainly be a part of future IPCC reports.

## Quantifying Uncertainty to Improve Model Predictions

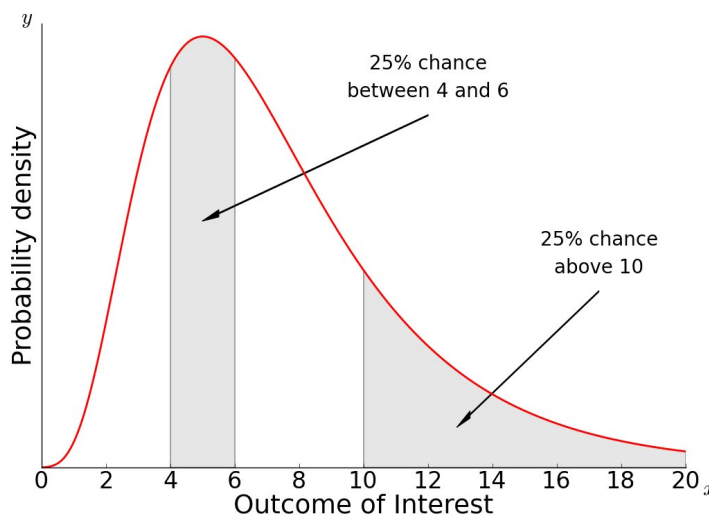
Another critical DOE objective is to enhance confidence in projections by both calibrating the model against historical observations and properly quantifying prediction uncertainties. UQ

is a relatively new science—enabled by the improved computational capabilities of the last decade—of quantifying the uncertainties in model inputs and predictions. With support from colleagues Bert Debusschere, Habib Najm, and Cosmin Safta, Khachik is leading the largest UQ effort in the ACME program.

Specifically, Khachik will be bounding uncertainties in predictions from land modeling, which focuses on the physical characteristics of vegetation, soil, and other terrestrial features at risk from climate

change. To explain how UQ comes into play, Khachik provides a simple example. "A single simulation of the land model may show that in 100 years, a certain type of vegetation will vanish. With UQ, we can actually quantify how likely it is to happen."

Instead of seeking a single result, UQ explores the range of findings provided by running the model multiple times—each time with different values for key parameters. The range of results can then be plotted, as in the simple graph shown above. Here, the x-axis shows the range of results for the outcome of interest, and the y-axis shows the probability density that each of the results might occur (that is, the area under the curve shows the likelihood that the outcome will be within a certain range of results).



*This simplified graph reflects a typical UQ result, revealing that outcome 5 is the mostly likely outcome to occur. The graph also demonstrates that the 25% chance of an outcome near 5 is the same as that for an outcome of greater than 10—defined here as a potentially catastrophic outcome.*

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## ACME: Climate Modeling Powered by DOE Supercomputers, Tamed by Uncertainty Quantification (cont'd)

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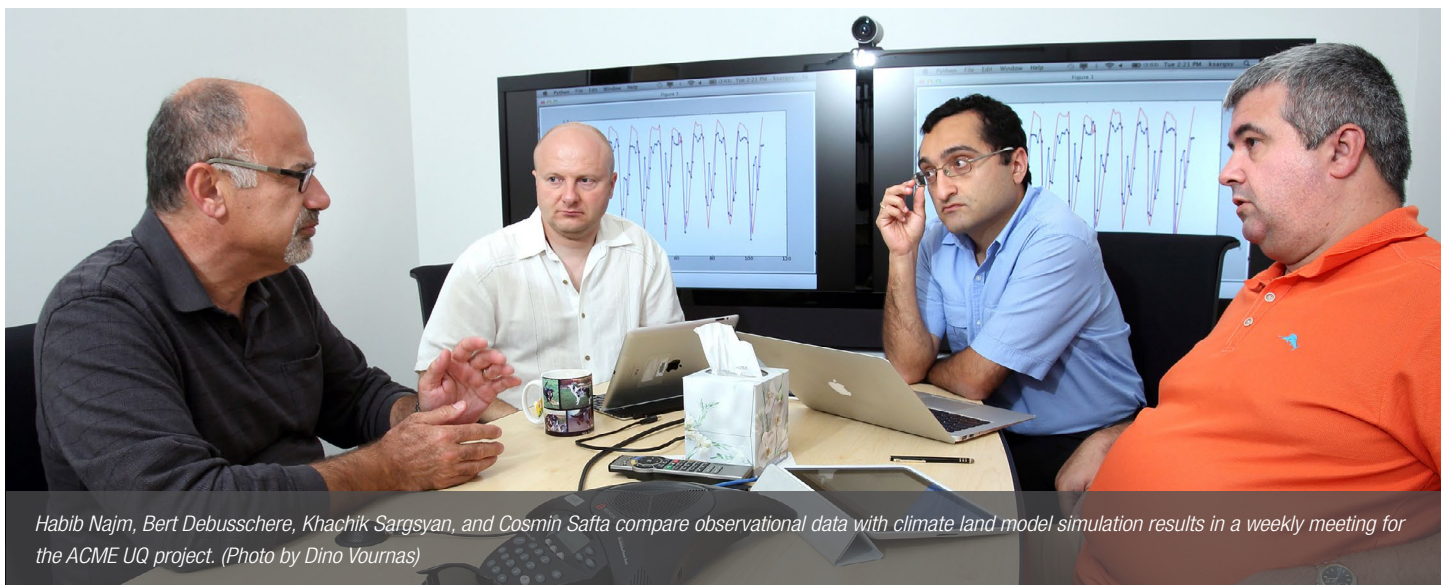
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"It's quite easy to see that result 5 is the mostly likely of all the results, but the grey areas under the curve add to the story. They show that there is a 25% probability that the true outcome is within the range of results between 4 and 6 and that there is a 25% chance that an outcome greater than 10 could occur," says Khachik.

In other words, the graph reveals there is a relatively low chance that the most likely outcome (or an outcome in its neighborhood) will materialize—a common result of UQ, says Khachik. "Graphs like these answer questions about the likeliness of an outcome and quantify associated risks. This information gives policy makers a very different understanding of model results, and hopefully allows them to formulate more effective policy."

model millions of times with millions of different input parameter settings. But given the size and complexity of climate change models, there simply isn't the budget for that," he says.

Instead, computational scientists employ advanced UQ methods to extract as much information about the model as possible, within a given computational budget. Khachik works closely with the land modeling partners from Oak Ridge National Laboratory (ORNL) to understand which parameters have the most impact on climate model outcomes and how exactly these parameters should be varied. "That way, you can run the model 100 times, rather than millions of times, and still get the answers you need to make reliable projections," he says.



*Habib Najm, Bert Debusschere, Khachik Sargsyan, and Cosmin Safta compare observational data with climate land model simulation results in a weekly meeting for the ACME UQ project. (Photo by Dino Vournas)*

This graph is one of the essential outcomes of the so-called forward UQ studies, where the variability in model inputs is propagated toward a range of variability in model outputs. The flip side of the coin is inverse UQ, in which one derives information on model input variability using actual observed historic data.

### Bounded by Computational Costs

Khachik explains that UQ is needed to assess the confidence in climate simulations—at reasonable cost. "Our research focuses on developing efficient algorithms for making UQ less expensive computationally. Ideally, to get the right answer, you would run the

With such limited model evaluations, UQ practitioners can then build a synthetic, surrogate approximation to the full climate model. This surrogate is typically computationally inexpensive to evaluate and replaces the full model with reasonable accuracy.

The UQ methods Khachik and his colleagues develop are notoriously nonintrusive—that is, they do not require programming changes to the original model (in this case, the climate model) that UQ is being applied to. Because of this important feature, UQ methods can be employed in a wide range of applications, from chemistry to materials science to nuclear engineering. It also means that previous efforts in different disciplines can expedite climate modeling UQ.

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## ACME: Climate Modeling Powered by DOE Supercomputers, Tamed by Uncertainty Quantification (cont'd)

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"As we grapple with climate modeling issues, my colleagues and I draw on intuition and formal mathematical machinery from previous UQ studies performed in the context of chemical models that have nothing to do with climate models," notes Khachik.

### Building Confidence in Results

Building trust that the scientific predictions are realistic and not biased by any political or social agenda may be the most important issue in motivating people and governments to take actions to address climate change, notes Chris. "Sandia's work in applying UQ to predictions of climate change is critical to establishing this trust. It shows that there is significant uncertainty in these projections, but that the uncertainty is bounded by realistic levels of probability."

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